

# On the Coupling of a Commercial Finite Element Package with LAMMPS for Multiscale Modeling of Materials

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**Abstract.** We present a semi-concurrent multiscale method to couple the commercial finite element package ABAQUS to the open source software LAMMPS. The coupling is implemented for static and dynamic applications. The semi-concurrent multiscale method here is based on the Cauchy-Born rule to compute stress/stiffness in continuum domain. It is realized through the ABAQUS user-interface UMAT and VUMAT. Implementation details are provided in this manuscript and the subroutines are made available at our homepage. One verification example is presented to show the validity of the coupling approach.

**Keywords:** Multiscale Analysis, Molecular Dynamics, Finite Element Analysis, LAMMPS

## 1. INTRODUCTION

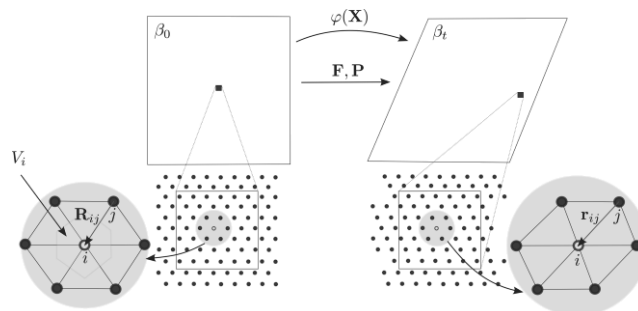
Nanoscience has been a rapidly growing science in the last two decades. Among various methodologies, molecular dynamics (MD) has gained exceptional success among others especially because of advances in the computational power. However, due to their high computational cost, MD simulations are restricted to specimen of small size. Therefore, multiscale methods have been developed to bridge different scales. In computational materials design, multiscale methods are powerful tools to extract material parameters based on fine-scale details. The  $FE^2$  method by Feyel *et. al* [1] is one of the most successful semi-concurrent multiscale method that accounts for fine-scale features on the coarse-scale. In this manuscript, we present a method to couple the commercial software package ABAQUS [2] to the open-source MD-software LAMMPS [3] through an  $FE^2$ -type method. An atomistic description is chosen on the fine-scale and a continuum model is used on the coarse-scale. In this manuscript, we restrict our studies to the Cauchy-Born (CB) bridging information from the atomistic scale to the continuum scale though the coupling is implemented for more general cases.

The implementation of (semi-)concurrent multiscale methods is a tedious task, particularly when either the MD-code or the FE-code has to be implemented from scratch. In this paper we try to bridge the gap between two well-known software for continuum and atomistic modeling in order to bring the method into a real-world application. This paper is organized as follows. First, the Cauchy-Born rule was presented briefly. Some implementation details are mentioned and then the numerical example is given to verify the method.

## 2. CAUCHY-BORN RULE

In the continuum-atomistic coupling, one approach is to replace the macroscopic strain energy density  $W_0$  per unit volume in the material configuration by appropriate atomistic potentials [4-6]. In the continuum-atomistic model, the important step is to find a correspondence between an atomistic energy function  $E_i$  and a specific strain energy density  $W_0$ . By the assumption that the individual atomic contributions to the total energy can be defined and that

the energy of each atom  $i$  is uniformly distributed over the volume  $V_i$  of its Voronoi polyhedron in Fig. 1, both energies can be related as follows [6]:



**Figure 1.** The 1<sup>st</sup>-order Cauchy-Born rule for the homogeneous deformation

$$W_0 \doteq \frac{E^{\text{int}}}{NV_i} = \frac{1}{NV_i} \sum_{i=1}^N E_i(r_{i1}, \dots, r_{iN}) = W_0(r_{i1}, \dots, r_{iN}) \quad (1)$$

where  $N$  is the number of atoms in the discrete lattice. For the establishment of a relation between atomic distance vectors and continuum deformation, 1<sup>st</sup>-order Cauchy-Born Rule (CBR) was used here. The idea of CBR comes from considering homogeneous deformations of an infinite representative crystallite. Suppose that  $\mathbf{r}_{ij}$  and  $\mathbf{R}_{ij}$  are lattice vectors in spatial and material coordinates and a deformation map  $\varphi(X)$  relates the material placement  $X$  to the spatial placement  $x = \varphi(X)$ . By defining  $F = \nabla_x \varphi$  as the local deformation gradient,

$$\mathbf{r}_{ij} = \mathbf{F} \cdot \mathbf{R}_{ij} \quad (2)$$

Combining Eq. (1) and Eq. (2), the strain energy density  $W_0$  can be expressed as a function of the fixed distance vectors in material coordinate and deformation gradient:

$$W_0 = W_0(r_{i1}, \dots, r_{iN}) = W_0(\mathbf{F} \cdot \mathbf{R}_{i1}, \dots, \mathbf{F} \cdot \mathbf{R}_{iN}) = W_0(\mathbf{F}) \quad (3)$$

Note that the distance vectors  $\mathbf{R}_{ij}$  in material coordinate depend only on initial geometrical crystal lattice structure. Therefore, each point of continuum domain can be modelled by an infinite crystal under homogeneous deformation. It should be mentioned that for pair potential, there is a cut-off radius  $r_c$  which limits the extension of crystal structure. In homogeneous deformation, the energies of all atoms are equivalent and hence, Eq. (1) can be written as:

$$W_0 = \frac{1}{NV_i} NE_i(r_{i1}, \dots, r_{iN}) = \frac{E_i(r_{i1}, \dots, r_{iN})}{V_i} = W_0(r_{i1}, \dots, r_{iN}) \quad (4)$$

From Eq. (4), it can be seen that for strain energy density in the entire lattice, the energy of one atom is sufficient. Furthermore, for pair potentials,  $W_0$  can be expressed in terms of interatomic pairwise interactions ( $\Phi_{ij}$ ):

$$W_0 = \frac{1}{2V_i} \sum_{j \neq i} \Phi_{ij} \quad (5)$$

In this case, the explicit constitutive law can be written as:

$$\begin{aligned} \mathbf{P} &= \frac{1}{NV_i} \sum_i \frac{\partial E_i}{\partial \mathbf{F}} \\ &= \frac{1}{N} \sum_i \frac{1}{2V_i} \sum_{j \neq i} \frac{E_{i,r_{ij}} + E_{j,r_{ji}}}{r_{ij}} \mathbf{r}_{ij} \otimes \mathbf{R}_{ij} \\ &= \frac{1}{N} \sum_i \frac{1}{2V_i} \sum_{j \neq i} \mathbf{f}_{ji} \otimes \mathbf{R}_{ij} \equiv \frac{1}{N} \sum_i \mathbf{P}_i \end{aligned} \quad (6)$$

where  $\mathbf{P}$  is 1<sup>st</sup> Piola-Kirchhoff stress tensor. Considering the relation between interatomic force,  $\mathbf{f}_{ji} = -\mathbf{f}_{ij}$ ,  $\mathbf{P}_i$  can be defined as:

$$\mathbf{P}_i \doteq \frac{1}{2V_i} \sum_{j \neq i} \mathbf{f}_{ji} \otimes \mathbf{R}_{ij} \quad (7)$$

In the case of the homogeneous deformation (standard Cauchy-Born rule),

$$\mathbf{P} = \frac{1}{N} N\mathbf{P}_i = \mathbf{P}_i \quad (8)$$

Similarly, the 4<sup>th</sup> tangent operator  $\mathbf{C}$  which relates the material rate of  $\mathbf{P}$  to the material rate of  $\mathbf{F}$ , can be expressed as:

$$\mathbf{C} \doteq \frac{\partial^2 W_0}{\partial \mathbf{F} \otimes \partial \mathbf{F}} \quad (9)$$

In the case of pair potentials the Eq. (9) can be simplified<sup>1</sup>:

$$\mathbf{C}_i = \frac{1}{2V_i} \sum_{j \neq i} \mathbf{k}_{ij} \overline{\otimes} [\mathbf{R}_{ij} \otimes \mathbf{R}_{ij}] \quad (10)$$

In this equation,  $\mathbf{k}_{ij}$  is the stiffness in atomic level and can be expressed as [7]:

$$\mathbf{k}_{ij} = \frac{\Phi'_{ij}}{r_{ij}} \mathbf{I} + \left[ \frac{\Phi''_{ij}}{r_{ij}^2} - \frac{\Phi'_{ij}}{r_{ij}^3} \right] \mathbf{r}_{ij} \otimes \mathbf{r}_{ij}, \quad i \neq j \quad (11)$$

For homogeneous deformation, the global tangent and the local tangent are equal:

$$\mathbf{C} = \frac{1}{N} N\mathbf{C}_i = \mathbf{C}_i \quad (12)$$

### 3. IMPLEMENTATION DETAILS

The connection between LAMMPS and ABAQUS was established through a Fortran2003 interface exploiting the ISOCBINDING module of Fortran 2003 standard. This interface allows accessing to many LAMMPS classes. A new "compute" was implemented into LAMMPS in C++ where it will compute the stress or material constitutive stiffness getting a deformation gradient with the Cauchy-Born rule. By using the deformation gradient from ABAQUS, the ABAQUS user material subroutine calls the compute command and gets back the stress/stiffness via the interface<sup>2</sup>. The lower-scale model is created with some LAMMPS commands input at the first time calling the material subroutine. For the subsequent calls, only the deformation gradient is changed and the compute command is called again. This way the overhead will be minimum for the multiscale model. This method is very flexible which can be used for many different potentials and material configuration. Moreover, the generality of the implementation allows for other homogenization methods to be used to extract the continuum properties.

### 4. NUMERICAL EXAMPLE

A three dimensional dog-bone specimen was used to test the multiscale method. Since the sections of the specimen which are in the grips does not have any strain, the distance between grips was considered in this study. Fig. 2 shows the model geometry and dimensions. Here, the metal unit system of LAMMPS was used in both scales. In this unit system, the distance unit is Angstroms, time unit is picoseconds, energy unit is eV, force unit is

<sup>1</sup> The non-standard dyadic product  $\overline{\otimes}$  for 2<sup>nd</sup>-order tensors is defined as  $[\mathbf{A} \overline{\otimes} \mathbf{B}] : \mathbf{C} = \mathbf{A} \cdot \mathbf{C} \cdot \mathbf{B}'$

<sup>2</sup> For more information about ABAQUS UMAT and Fortran interface, please visit the following website: <https://sites.google.com/site/permixproject/lammmps2f03>

eV/Angstrom, pressure unit is bars and mass unit is grams/mole. The simulation was conducted using a displacement control method and due to symmetry, only a one eighth of specimen was simulated, Fig. 3. For the underlying material model, a small FCC lattice with the lattice parameter 3.645 Å is defined. The inter-atomic forces are described with the Lennard-Jones (LJ) potential:

$$\Phi_{LJ} = 4\epsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right] \quad (13)$$

where  $\epsilon$  is the depth of the potential well and  $\sigma$  is the finite distance at which the inter-particle potential is zero. For this simulation, the LJ potential parameters are selected as  $\sigma = 2.29621$  and  $\epsilon = 0.467$ . These parameters are correspondent to those of Copper. Though in general, the LJ potential is not very suitable for modeling metals. Nevertheless, the LJ potential can fairly represent the overall material behaviour in the atomistic scale and often researchers use it to show some conceptual phenomena rather than real material behavior [8–10]. Only nearest neighbour interactions are considered here. Fig. 4 shows the von-Mises stress contour.

The general coupling procedure of the two software can be applied to any type of material which can be handled by LAMMPS in the fine scale and ABAQUS in the coarse scale. However, since we used the Cauchy-Born rule here to compute the homogenized material properties, the current implementation can be used for materials that can be modeled by pair potentials such as Lennard-Jones, Embedded Atom Method (EAM), Modified Embedded Atom Method (MEAM), etc. The last two potential are very much suitable to model metals such as steel and copper [11, 12]. Using another homogenization procedure such as the  $FE^2$  method [1], this implementation can be further used to model materials from Macro-Meso-Scale with the Peridynamic capability of LAMMPS [13].

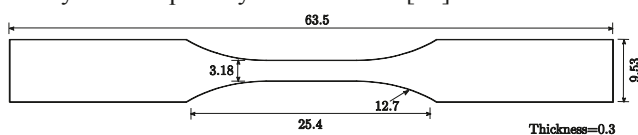


Figure 2. The dimensions of dog-bone sample

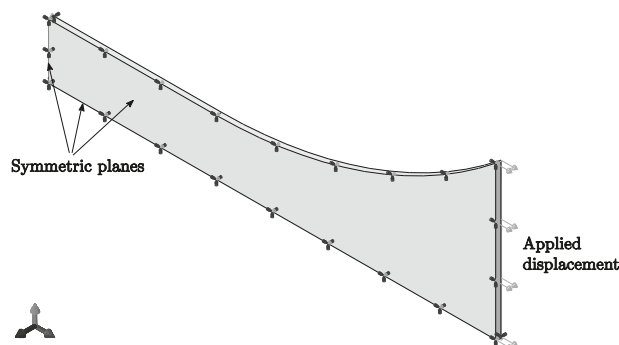


Figure 3. The initial dog-bone configuration

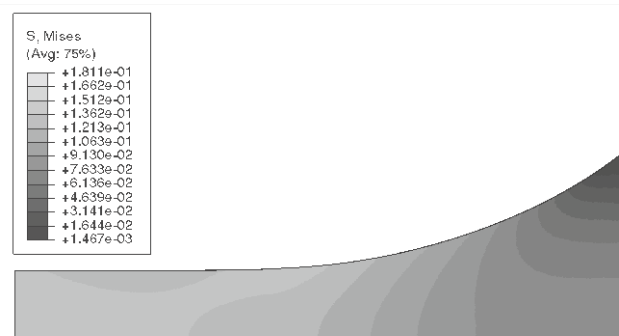


Figure 4. The von-Mises stress contour

Fig. 5 shows the stress-strain curve for a highly stress integration point. As it can be observed from Fig. 5, the material undergoes strain softening after 11% of strain.

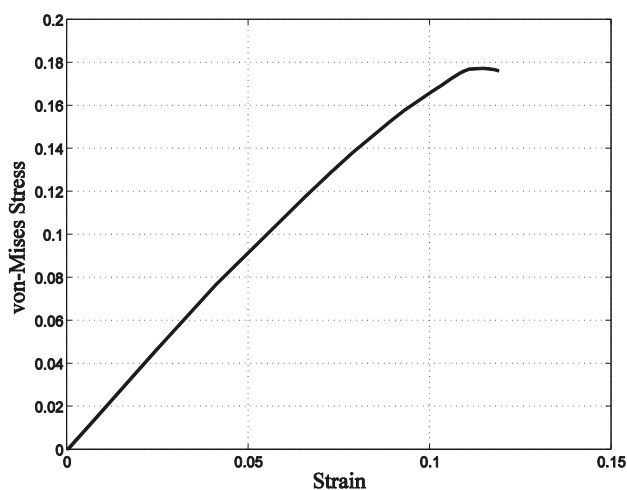


Figure 5. The plot of stress versus strain for an integration point with maximum stress

## 5. CONCLUSION

Based on a semi-concurrent multiscale method, we coupled the FE-software package ABAQUS with the MD-software LAMMPS. Using the user material subroutines of ABAQUS at every Gauss point, the deformation gradient of the continuum domain was transferred to the atomistic software (LAMMPS). The Cauchy-Born rule was used to calculate the stress tensor and the consistent material tangent stiffness tensor from the atomistic model. We presented one example, a dog-bone specimen under uni-axial tension and used the LJ-potential on atomistic scale to show the validity of the method. In the future, we will extend the method to more complex potentials, fracture [14-17], meshfree methods [18] and large deformations [19].

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